



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:53 AM UTC

PDB ID : 6I1H / pdb_00006i1h
Title : Crystal structure of TP domain from Chlamydia trachomatis Penicillin-Binding Protein 3 in complex with meropenem
Authors : Bellini, D.; Koekemoer, L.; Newman, H.; Dowson, C.G.
Deposited on : 2018-10-28
Resolution : 1.78 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

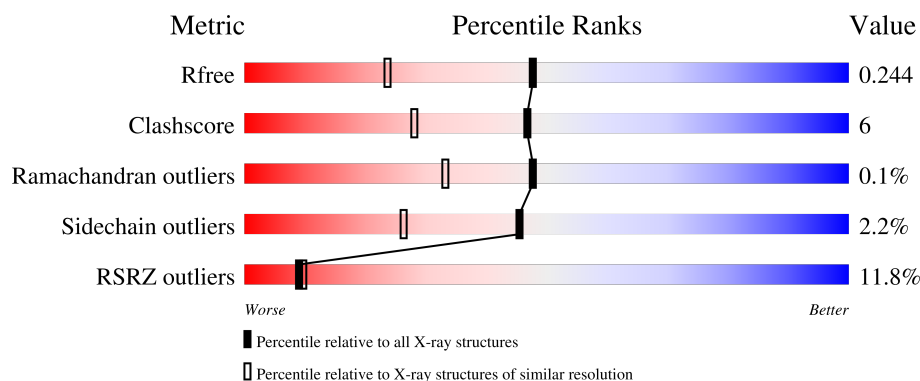
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	346	6% 88% 9% ..
1	B	346	17% 83% 13% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5241 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

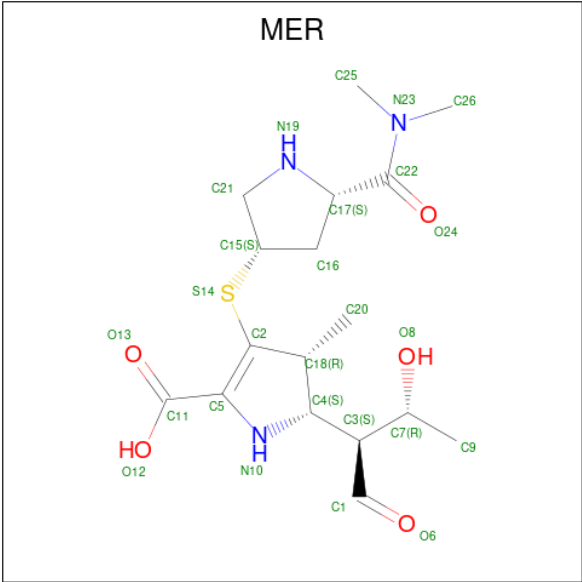
- Molecule 1 is a protein called Penicillin-binding protein, Penicillin-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2519	1581	426	503	9			
1	B	336	Total	C	N	O	S	0	0	0
			2492	1566	421	496	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	256	GLY	-	expression tag	UNP A0A0E9FXJ8
A	257	PRO	-	expression tag	UNP A0A0E9FXJ8
A	258	GLY	-	expression tag	UNP A0A0E9FXJ8
A	259	TYR	-	expression tag	UNP A0A0E9FXJ8
A	260	GLN	-	expression tag	UNP A0A0E9FXJ8
A	261	ASP	-	expression tag	UNP A0A0E9FXJ8
A	262	PRO	-	expression tag	UNP A0A0E9FXJ8
A	306	PRO	-	linker	UNP A0A0E9FXJ8
A	307	GLY	-	linker	UNP A0A0E9FXJ8
B	256	GLY	-	expression tag	UNP A0A0E9FXJ8
B	257	PRO	-	expression tag	UNP A0A0E9FXJ8
B	258	GLY	-	expression tag	UNP A0A0E9FXJ8
B	259	TYR	-	expression tag	UNP A0A0E9FXJ8
B	260	GLN	-	expression tag	UNP A0A0E9FXJ8
B	261	ASP	-	expression tag	UNP A0A0E9FXJ8
B	262	PRO	-	expression tag	UNP A0A0E9FXJ8
B	306	PRO	-	linker	UNP A0A0E9FXJ8
B	307	GLY	-	linker	UNP A0A0E9FXJ8

- Molecule 2 is (4R,5S)-3-([(3S,5S)-5-(dimethylcarbamoyl)pyrrolidin-3-yl]sulfanyl)-5-[(2S,3R)-3-hydroxy-1-oxobutan-2-yl]-4-methyl-4,5-dihydro-1H-pyrrole-2-carboxylic acid (CCD ID: MER) (formula: C₁₇H₂₇N₃O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	17	3	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	17	3	5	1		

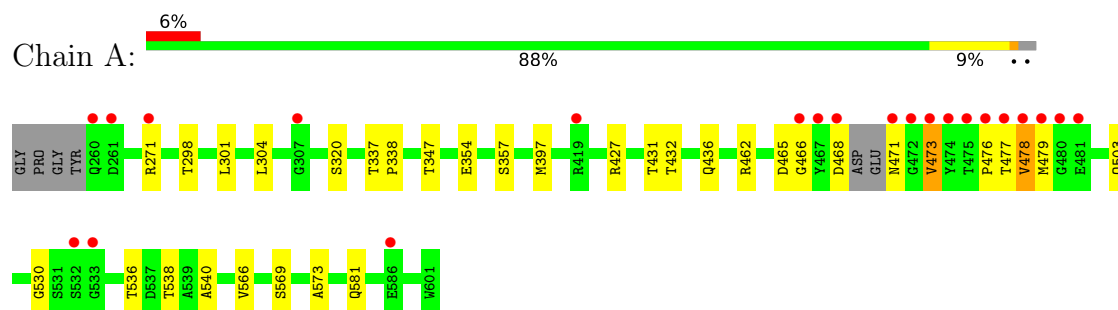
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total	O	0	0
			119	119		
3	B	59	Total	O	0	0
			59	59		

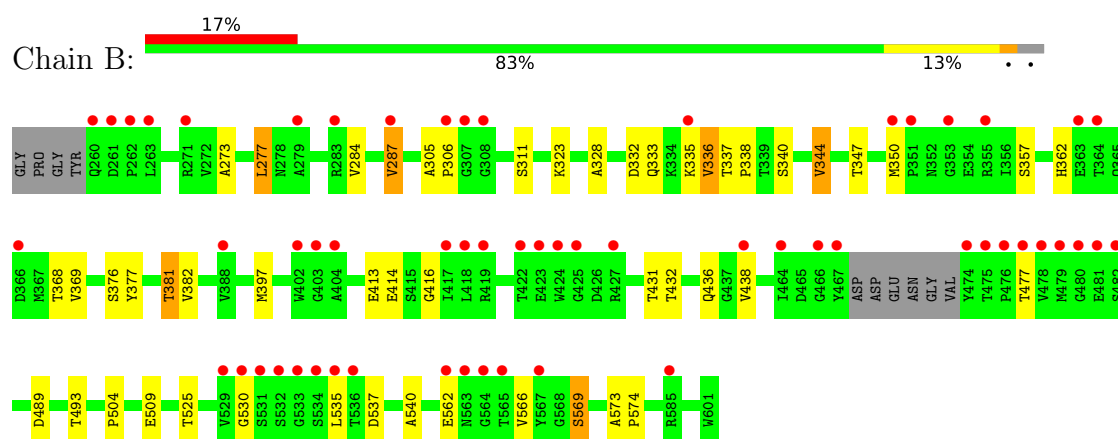
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Penicillin-binding protein, Penicillin-binding protein



- Molecule 1: Penicillin-binding protein, Penicillin-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.57Å 112.57Å 118.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.49 – 1.78 97.48 – 1.78	Depositor EDS
% Data completeness (in resolution range)	64.0 (97.49-1.78) 64.0 (97.48-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.221 , 0.251 0.212 , 0.244	Depositor DCC
R_{free} test set	2579 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5241	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MER

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.66	1/2567 (0.0%)	0.82	0/3500
1	B	0.60	0/2540	0.84	1/3463 (0.0%)
All	All	0.63	1/5107 (0.0%)	0.83	1/6963 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	538	THR	C-O	-5.01	1.18	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	477	THR	N-CA-C	5.20	117.57	110.55

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2519	0	2496	26	0
1	B	2492	0	2473	31	0
2	A	26	0	26	5	0
2	B	26	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	119	0	0	1	0
3	B	59	0	0	5	0
All	All	5241	0	5020	57	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (57) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:SER:OG	2:A:701:MER:C1	1.75	1.34
1:A:320:SER:OG	2:A:701:MER:H1	0.93	1.08
1:A:320:SER:CB	2:A:701:MER:H1	2.12	0.78
1:A:320:SER:HG	2:A:701:MER:H1	0.94	0.76
1:A:471:ASN:HB2	1:A:473:VAL:HG22	1.67	0.76
1:B:377:TYR:O	1:B:381:THR:HG23	1.87	0.74
1:B:540:ALA:HB2	1:B:566:VAL:HG13	1.74	0.69
1:B:574:PRO:O	3:B:802:HOH:O	2.11	0.68
1:A:337:THR:HB	1:A:338:PRO:HD2	1.74	0.67
1:A:581:GLN:HG2	3:A:885:HOH:O	1.93	0.67
1:B:344:VAL:CG1	1:B:362:HIS:HE1	2.12	0.62
1:B:431:THR:HB	1:B:436:GLN:HB3	1.81	0.62
1:B:350:MET:HE3	1:B:382:VAL:HG21	1.81	0.61
1:B:311:SER:CB	3:B:801:HOH:O	2.46	0.59
1:B:311:SER:N	3:B:801:HOH:O	1.66	0.58
1:B:489:ASP:O	1:B:493:THR:HG23	2.02	0.58
1:B:305:ALA:HB1	1:B:306:PRO:HA	1.86	0.57
1:A:320:SER:CB	2:A:701:MER:C1	2.78	0.57
1:B:344:VAL:HG12	1:B:362:HIS:HE1	1.69	0.57
1:A:397:MET:HE1	1:A:432:THR:HB	1.88	0.55
1:B:284:VAL:HG11	1:B:566:VAL:HG21	1.88	0.54
1:B:413:GLU:HG3	3:B:804:HOH:O	2.07	0.54
1:B:336:VAL:HG13	1:B:369:VAL:HG21	1.89	0.53
1:B:287:VAL:HG21	1:B:562:GLU:HG3	1.91	0.52
1:A:354:GLU:OE2	1:A:427:ARG:HD2	2.09	0.51
1:A:301:LEU:HD21	1:A:304:LEU:HB2	1.92	0.51
1:B:273:ALA:O	1:B:277:LEU:HB2	2.10	0.51
1:A:466:GLY:HA2	1:A:477:THR:HG23	1.94	0.50
1:A:466:GLY:HA3	1:A:476:PRO:HA	1.94	0.50
1:B:284:VAL:HG11	1:B:566:VAL:CG2	2.43	0.49
1:A:271:ARG:HG3	3:B:849:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ASP:HA	1:A:473:VAL:O	2.13	0.48
1:B:397:MET:HE1	1:B:432:THR:HB	1.95	0.48
1:B:530:GLY:HA3	1:B:537:ASP:OD2	2.13	0.48
1:B:333:GLN:HB3	1:B:335:LYS:HD2	1.97	0.47
1:A:478:VAL:HG12	1:A:479:MET:H	1.79	0.47
1:B:323:LYS:HD3	1:B:381:THR:HG21	1.97	0.47
1:B:569:SER:O	1:B:573:ALA:HB3	2.15	0.47
1:A:301:LEU:HD11	1:A:304:LEU:HD13	1.96	0.46
1:A:431:THR:HB	1:A:436:GLN:HB2	1.97	0.46
1:A:462:ARG:NH1	1:A:479:MET:HA	2.32	0.45
1:A:540:ALA:HB2	1:A:566:VAL:HG23	1.99	0.45
1:B:344:VAL:HG11	1:B:377:TYR:CD2	2.51	0.45
1:B:347:THR:HG22	1:B:357:SER:HB3	1.98	0.45
1:A:301:LEU:HD21	1:A:304:LEU:HD22	1.98	0.44
1:A:298:THR:O	1:A:462:ARG:NH1	2.51	0.44
1:A:347:THR:HG22	1:A:357:SER:HB3	2.00	0.44
1:B:337:THR:HB	1:B:338:PRO:CD	2.48	0.44
1:B:414:GLU:HG3	1:B:416:GLY:H	1.83	0.44
1:B:328:ALA:O	1:B:332:ASP:HB2	2.18	0.43
1:A:337:THR:HB	1:A:338:PRO:CD	2.43	0.43
1:B:340:SER:O	1:B:368:THR:HA	2.18	0.43
1:A:530:GLY:HA3	1:A:536:THR:OG1	2.20	0.42
1:A:569:SER:O	1:A:573:ALA:HB3	2.20	0.42
1:B:504:PRO:HA	1:B:509:GLU:CD	2.46	0.41
1:B:525:THR:HG23	1:B:566:VAL:O	2.20	0.41
1:B:350:MET:CE	1:B:382:VAL:HG21	2.46	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/346 (97%)	330 (98%)	6 (2%)	0	100	100
1	B	332/346 (96%)	325 (98%)	6 (2%)	1 (0%)	36	22
All	All	668/692 (96%)	655 (98%)	12 (2%)	1 (0%)	48	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	535	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/273 (98%)	265 (98%)	4 (2%)	57	41
1	B	266/273 (97%)	258 (97%)	8 (3%)	36	15
All	All	535/546 (98%)	523 (98%)	12 (2%)	45	26

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	465	ASP
1	A	473	VAL
1	A	478	VAL
1	A	503	GLN
1	B	277	LEU
1	B	287	VAL
1	B	336	VAL
1	B	344	VAL
1	B	376	SER
1	B	381	THR
1	B	438	VAL
1	B	569	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	GLN
1	A	383	GLN
1	B	362	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	MER	B	701	-	22,27,27	1.03	1 (4%)	20,39,39	1.11	2 (10%)
2	MER	A	701	-	22,27,27	1.17	1 (4%)	20,39,39	1.48	3 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MER	B	701	-	-	7/23/51/51	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MER	A	701	-	-	6/23/51/51	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	MER	C15-S14	-4.41	1.76	1.82
2	B	701	MER	C15-S14	-3.16	1.78	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	MER	C18-C4-N10	-3.54	102.34	105.07
2	A	701	MER	C5-C2-S14	3.45	129.22	124.37
2	A	701	MER	O12-C11-C5	2.85	121.25	116.73
2	B	701	MER	O12-C11-C5	2.42	120.56	116.73
2	B	701	MER	O6-C1-C3	-2.10	120.25	125.27

There are no chirality outliers.

All (13) torsion outliers are listed below:

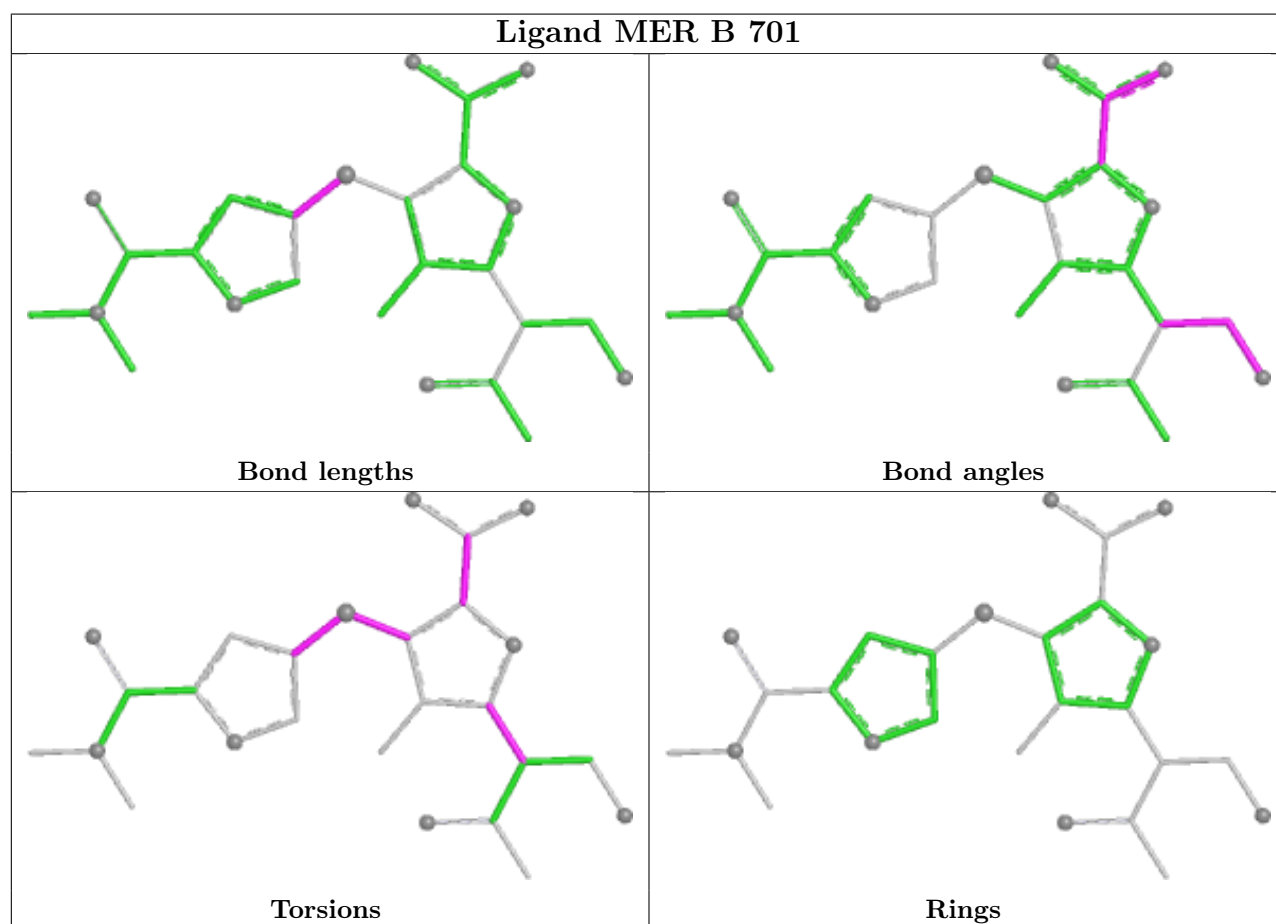
Mol	Chain	Res	Type	Atoms
2	A	701	MER	C5-C2-S14-C15
2	A	701	MER	C7-C3-C4-C18
2	A	701	MER	O12-C11-C5-C2
2	A	701	MER	O13-C11-C5-C2
2	A	701	MER	O12-C11-C5-N10
2	A	701	MER	O13-C11-C5-N10
2	B	701	MER	C5-C2-S14-C15
2	B	701	MER	C7-C3-C4-C18
2	B	701	MER	O12-C11-C5-C2
2	B	701	MER	O13-C11-C5-C2
2	B	701	MER	O12-C11-C5-N10
2	B	701	MER	O13-C11-C5-N10
2	B	701	MER	C21-C15-S14-C2

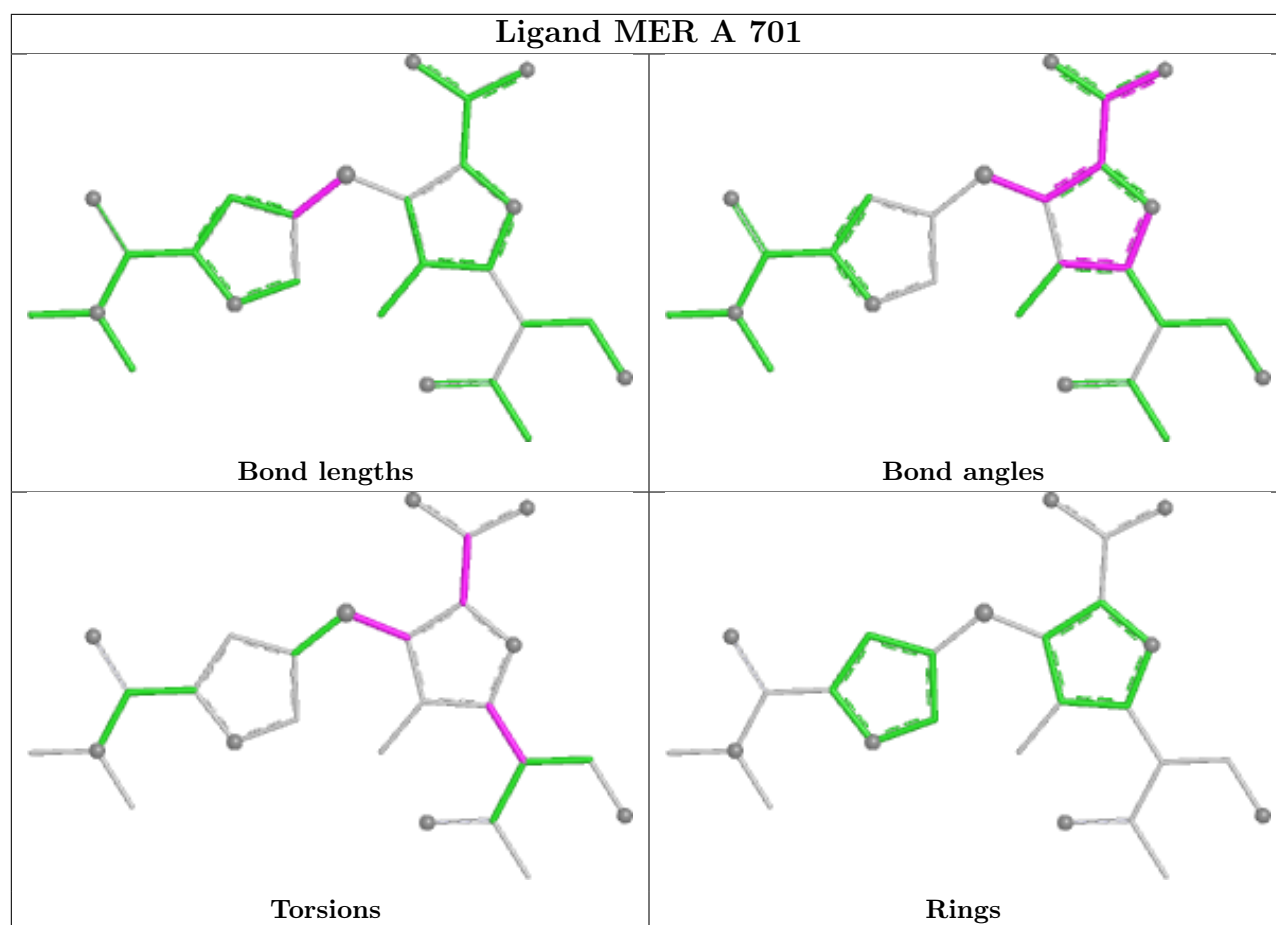
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	MER	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	340/346 (98%)	0.14	22 (6%) 25 30	9, 17, 42, 64	0
1	B	336/346 (97%)	0.99	58 (17%) 4 4	14, 28, 59, 92	0
All	All	676/692 (97%)	0.57	80 (11%) 9 10	9, 21, 53, 92	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	478	VAL	11.2
1	A	467	TYR	8.3
1	A	473	VAL	6.6
1	A	478	VAL	6.3
1	B	535	LEU	5.6
1	B	529	VAL	5.4
1	A	260	GLN	5.3
1	A	475	THR	5.2
1	B	533	GLY	5.2
1	B	531	SER	5.2
1	B	530	GLY	5.1
1	B	534	SER	5.1
1	A	476	PRO	5.1
1	B	260	GLN	4.6
1	B	261	ASP	4.5
1	B	467	TYR	4.3
1	B	474	TYR	4.3
1	B	466	GLY	4.1
1	B	532	SER	4.1
1	A	480	GLY	4.0
1	A	474	TYR	4.0
1	A	479	MET	3.9
1	A	419	ARG	3.8
1	B	307	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	424	TRP	3.7
1	B	567	TYR	3.7
1	B	422	THR	3.7
1	B	427	ARG	3.6
1	B	480	GLY	3.5
1	A	466	GLY	3.4
1	B	476	PRO	3.3
1	B	565	THR	3.2
1	A	477	THR	3.2
1	A	471	ASN	3.1
1	B	388	VAL	3.1
1	A	472	GLY	3.0
1	B	419	ARG	2.9
1	B	306	PRO	2.9
1	A	271	ARG	2.9
1	B	335	LYS	2.9
1	B	475	THR	2.9
1	B	353	GLY	2.8
1	B	418	LEU	2.8
1	A	468	ASP	2.8
1	A	532	SER	2.8
1	B	479	MET	2.8
1	B	402	TRP	2.7
1	B	481	GLU	2.7
1	B	562	GLU	2.7
1	B	425	GLY	2.7
1	B	262	PRO	2.7
1	B	482	SER	2.7
1	B	417	ILE	2.6
1	B	536	THR	2.6
1	B	263	LEU	2.6
1	B	363	GLU	2.5
1	A	586	GLU	2.5
1	B	563	ASN	2.4
1	B	271	ARG	2.4
1	B	279	ALA	2.4
1	B	585	ARG	2.4
1	B	350	MET	2.4
1	B	351	PRO	2.3
1	A	533	GLY	2.3
1	B	423	GLU	2.3
1	A	261	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	481	GLU	2.3
1	B	464	ILE	2.3
1	B	287	VAL	2.3
1	B	438	VAL	2.1
1	B	355	ARG	2.1
1	B	366	ASP	2.1
1	A	307	GLY	2.1
1	B	364	THR	2.1
1	B	283	ARG	2.1
1	B	477	THR	2.1
1	B	308	GLY	2.0
1	B	403	GLY	2.0
1	B	564	GLY	2.0
1	B	404	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

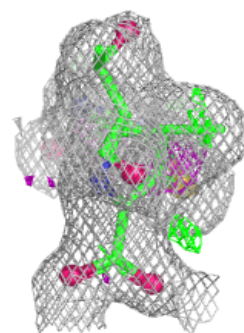
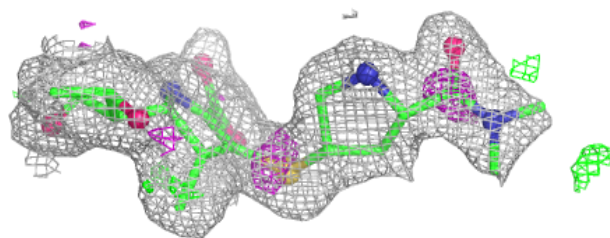
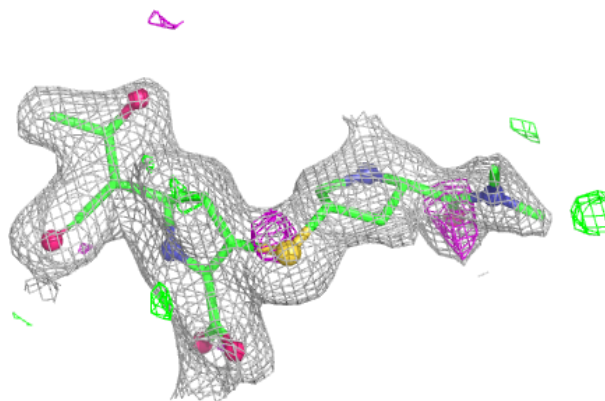
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MER	B	701	26/26	0.85	0.14	33,37,40,41	0
2	MER	A	701	26/26	0.96	0.06	13,14,17,17	0

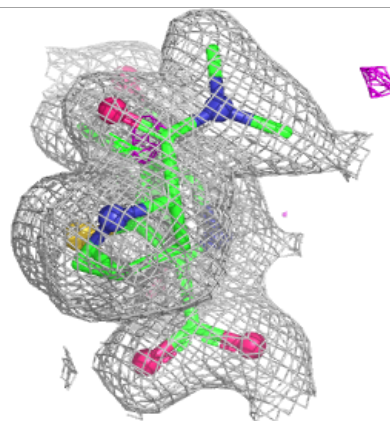
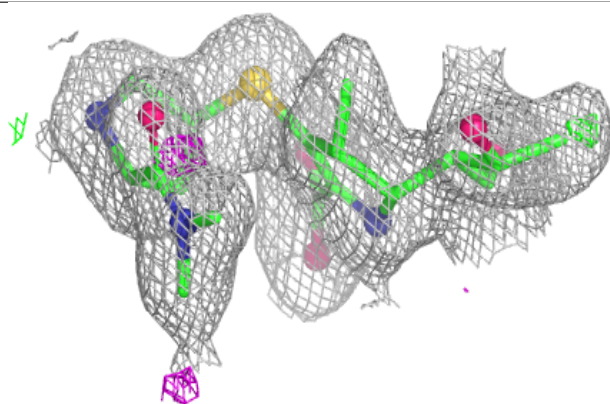
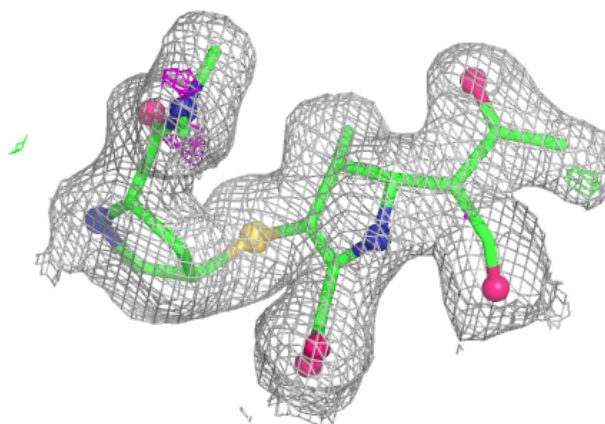
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MER B 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around MER A 701:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.